High Performance Computing Requirements- A Remote User's Perspective

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Outline

- Background
- Remote Computing Issues
- Remote Graphics
- Balancing Hardware and Software

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Background

- **Areas Of Interest**
  - **Computational Fluid Dynamics**
  - **Code Parallelization**
  - **Scientific Visualization**
- **CFD Work With SHAMRC**
  - **Second-order Hydrodynamic Adaptive Mesh Refinement Code**
- **Experience With LANL And DoD HPC Sites**
  - **DTRA**

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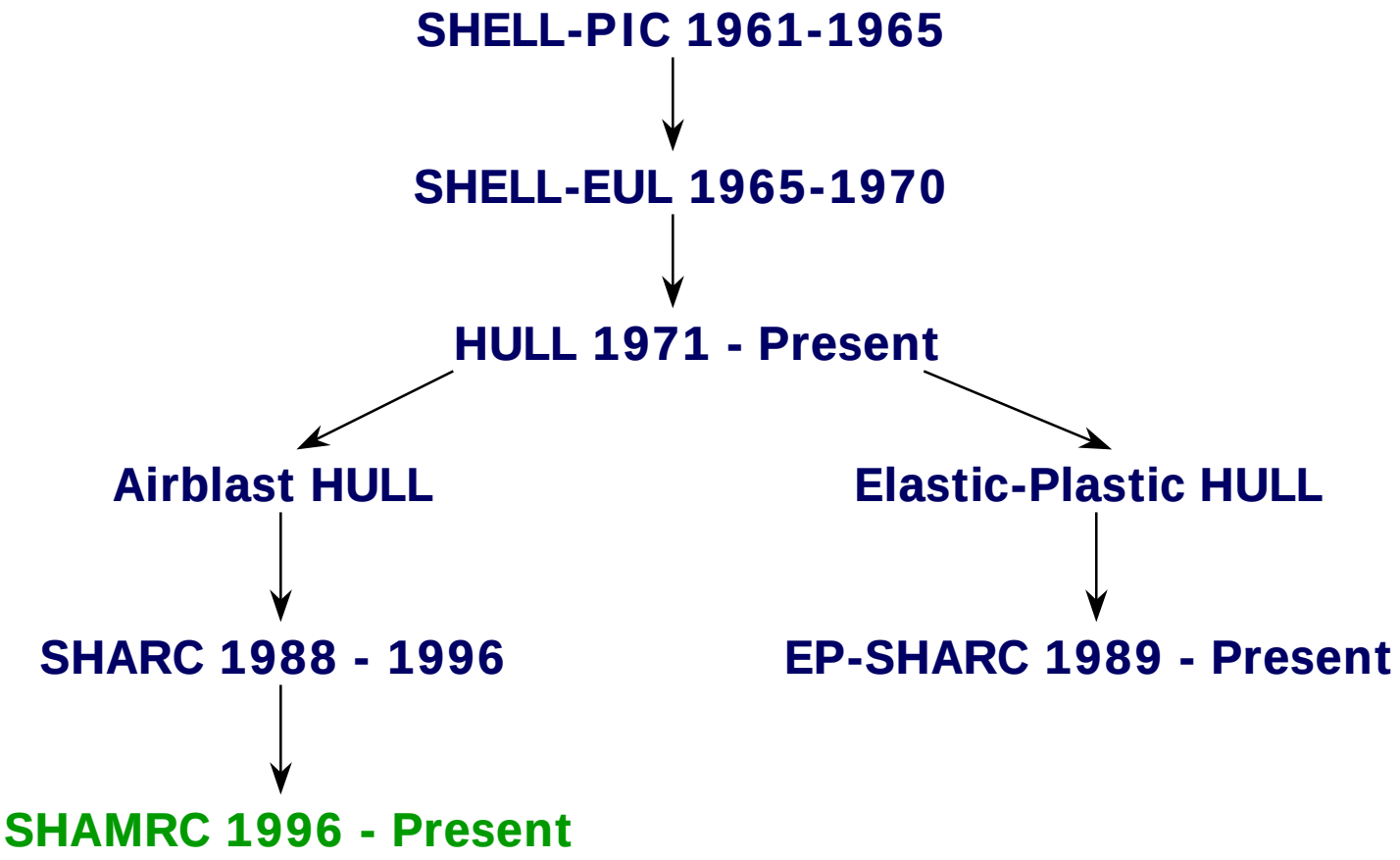
SHAMRC History



Attributes

- Eulerian Differencing Scheme
- Second-Order Accurate in Both Space and Time
- Fully Conservative of Mass, Momentum, and Energy
- Adaptive Mesh Refinement
- Parallel (Single-grid and AMR)
- Rich Set Of Models
  - Turbulence Model
  - HE Detonations
  - Interactive Particulates
  - Etc.

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Sample Applications

- **Typical Problems**
  - **50 – 200 Million Cells**
  - **1 – 4 Gbyte Restart files**
  - **100 – 500 Hours Wallclock Time**
- **Vehicle Loads From the LB/TS Exit Jet**
- **Blast Wall Evaluation**
- **Blast Loads on Buildings**
- **Oklahoma City**

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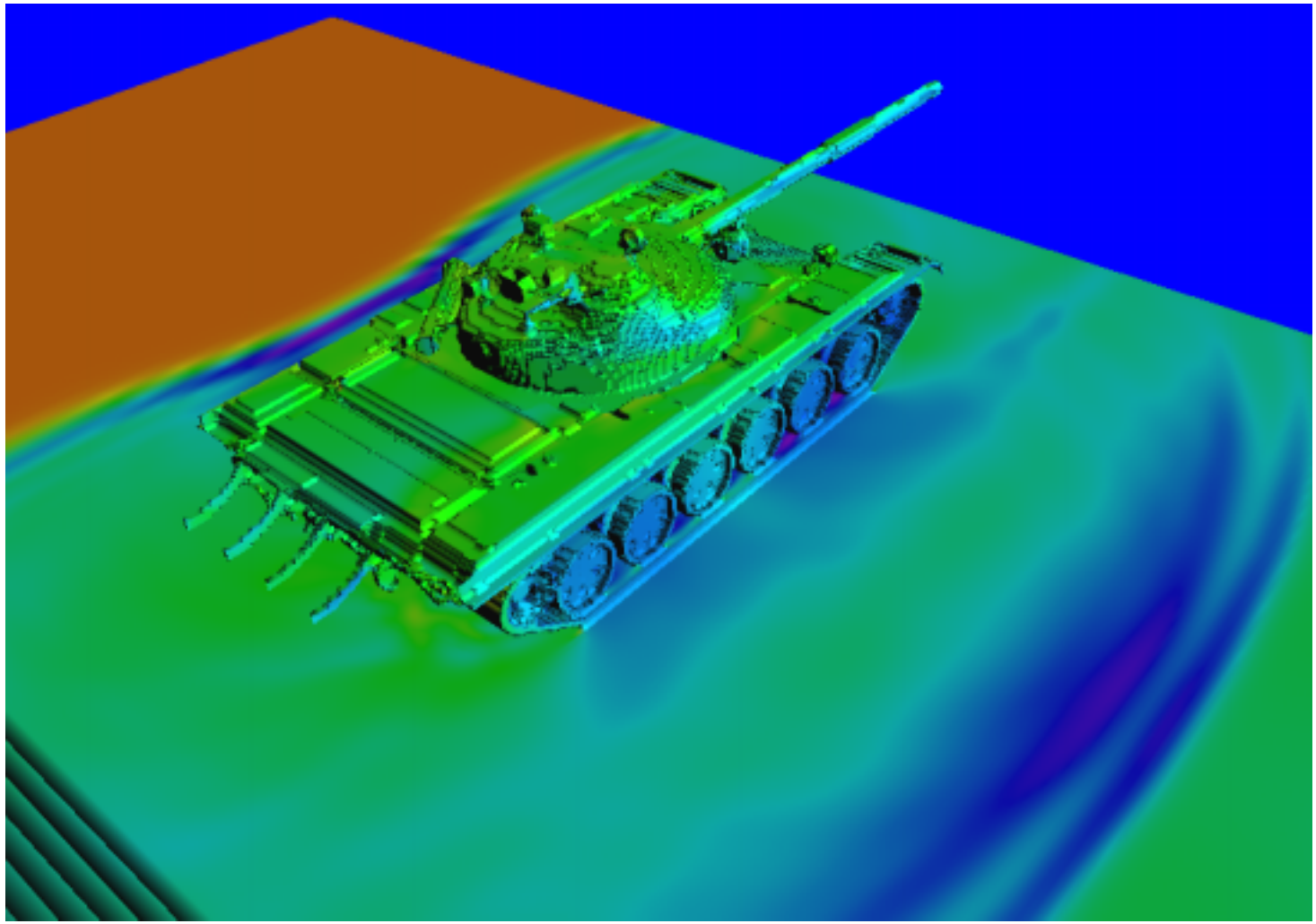
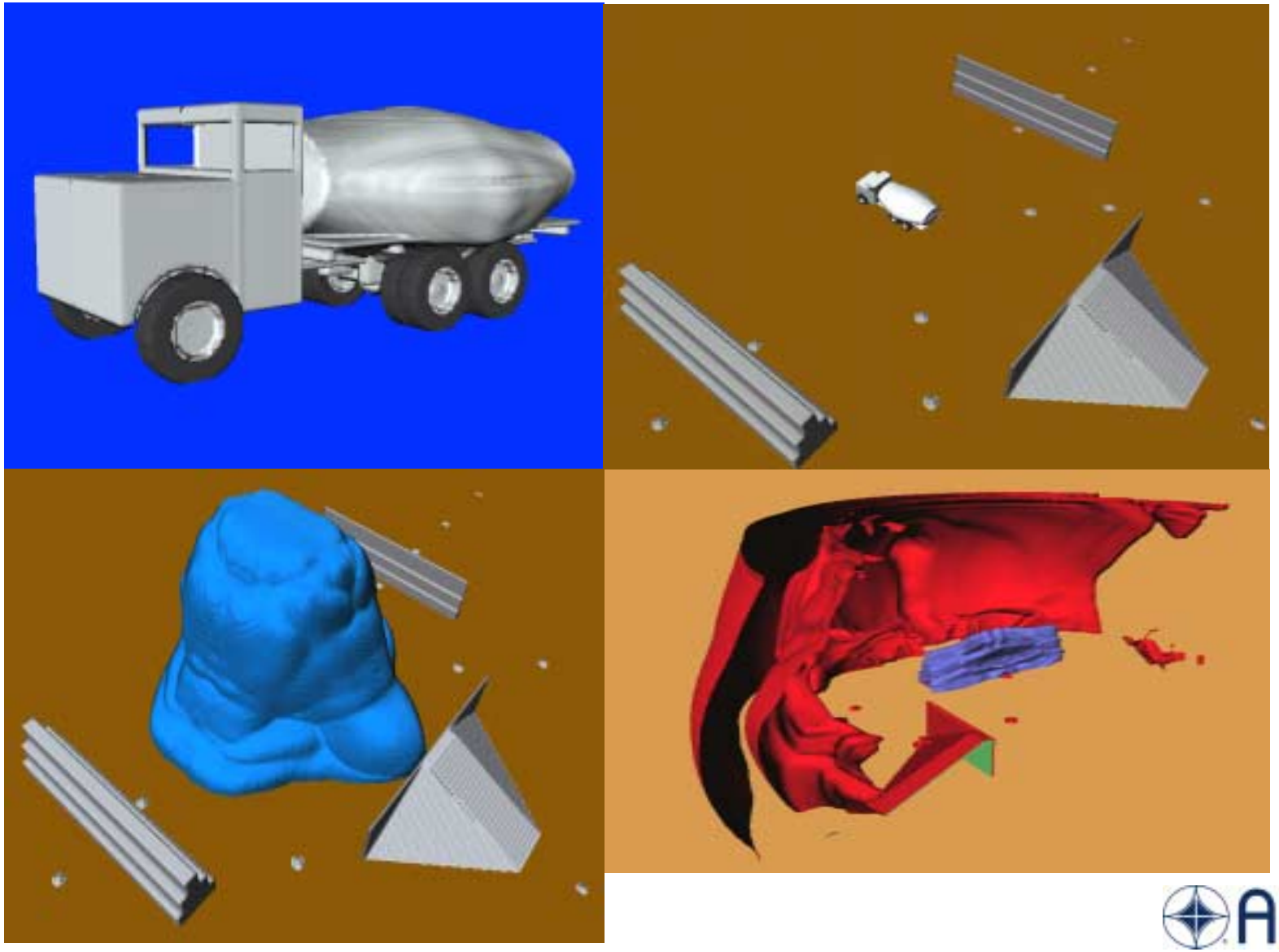
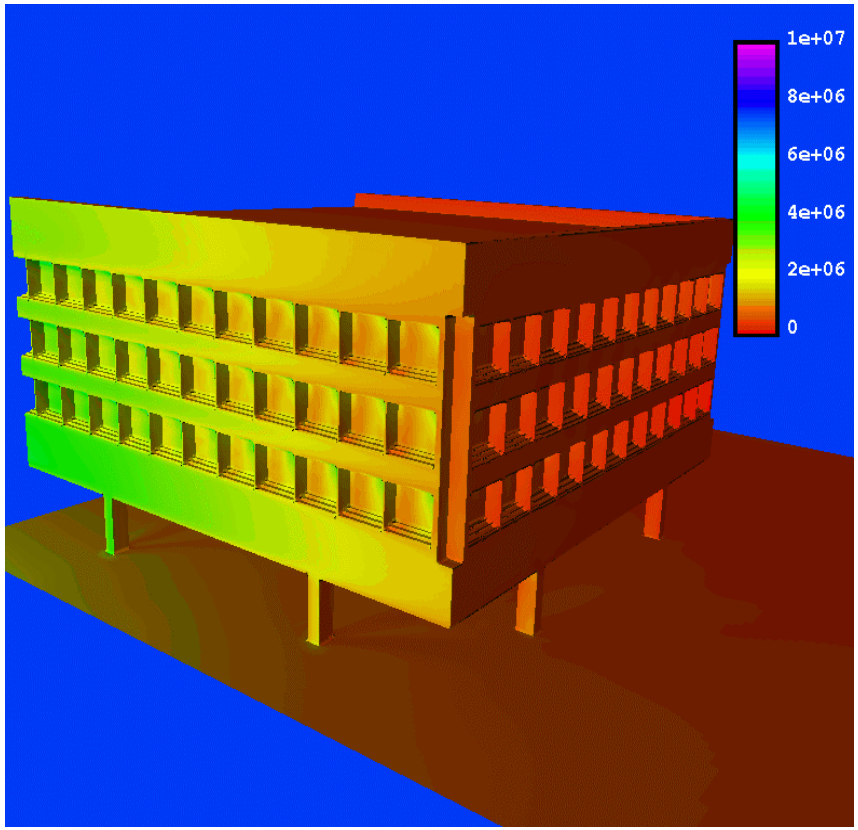
LB/TS Vehicle Load Calculation



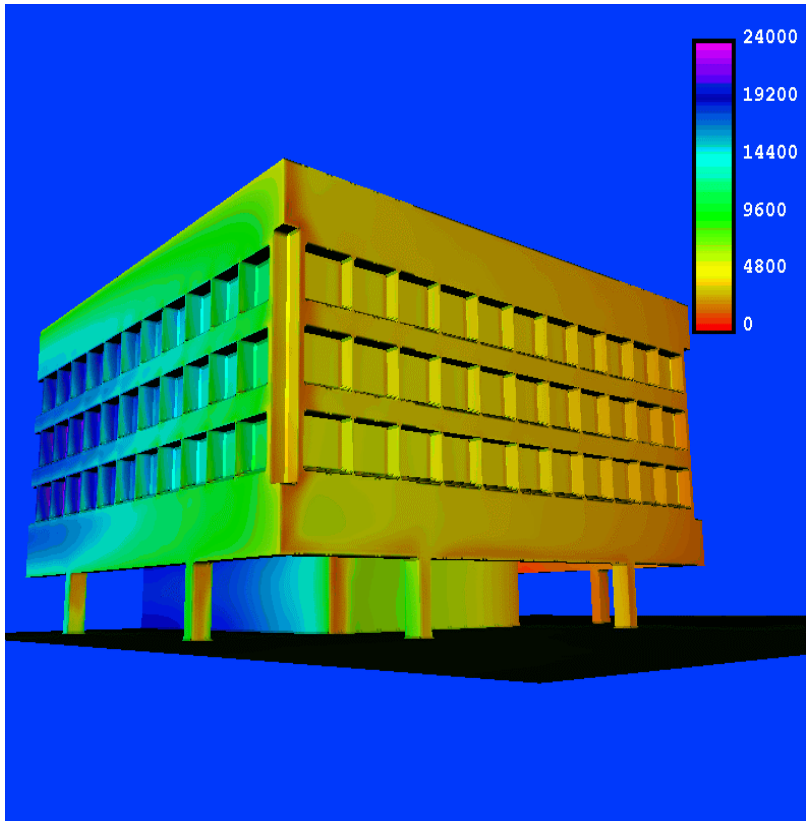
Detonation And Airblast Propagation From A Truck Bomb



Airblast Loads on Buildings

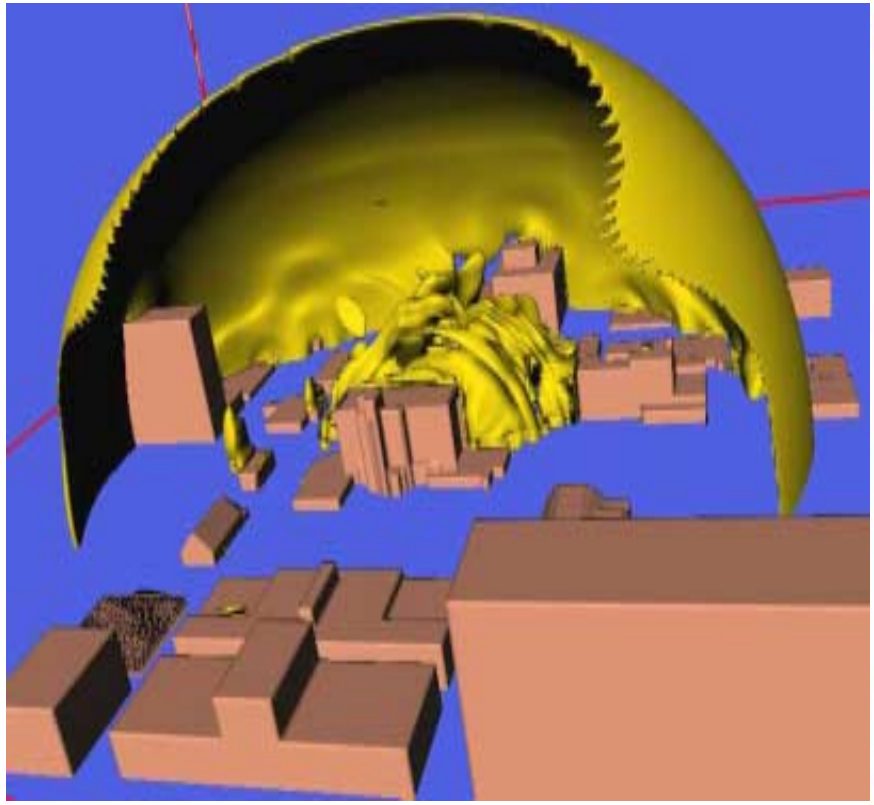


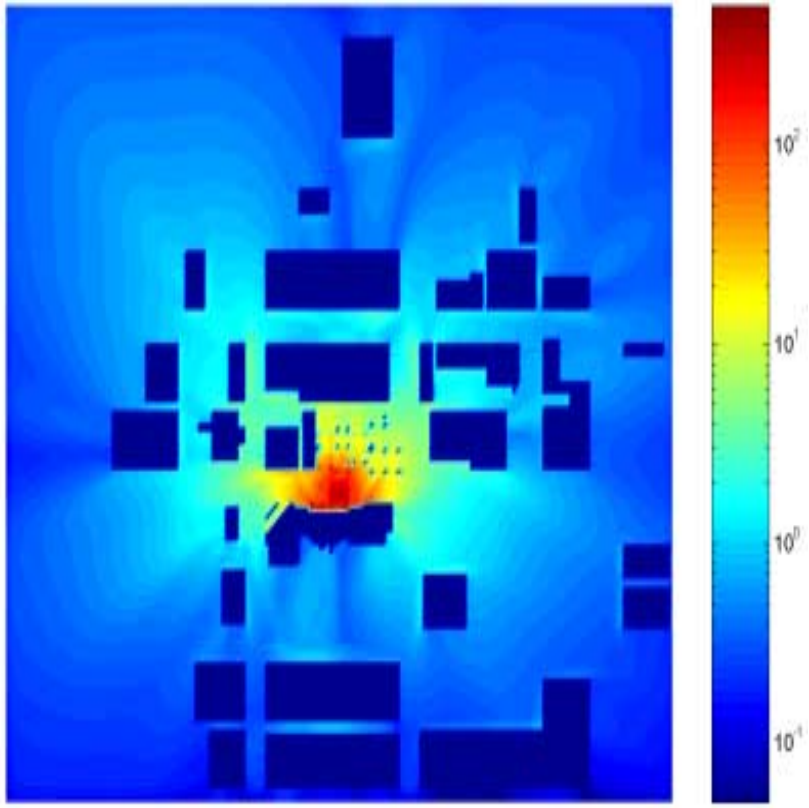
Peak Overpressure



Peak Overpressure Impulse

Oklahoma City Blast Evaluation





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HPC Requirements

+ **Lots Of Fast CPUs**
+ **Memory**
+ **Online/Offline Storage**
+ **Reliability**
+ **Software (Debuggers, Graphics, etc.)**
+ **User Support**
+ **Serial Processing Capability**

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Remote Computing Issues

- **Communications Issues – The Problem Is Not in Running The Calculations, It Is Processing the Results**
  - **Bandwidth**
    - **Need More**
  - **Kerberos, SSH**
    - **Stabilize and Standardize**
  - **Firewalls**
  - **File Transfers (Ftp, Scp, …)**
  - **X-based Applications**
    - **Tooooooo Slooooooow**
- **Access to Training**
- **3D Graphics Capabilities**

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Communications Issues

- **Remote Computing Happens at a Slower Pace Than On-site Computing**
  - **Not the Computing Itself, but All the Other Aspects Related to Scientific Computing**
    - **File Transfers, Post-processing, Debugging, …**
- **The Main Reason – Bandwidth**
- **Typical Access Via a T1**
  - **Shared With Many Users**

Communications Issues

- **Kerberos And Ssh**
  - **Changed On A Weekly Basis For The First Year**
    - **What Is The Access Method Of The Week**
  - **Inconsistent Use From Site To Site**
    - **Between LANL And DoD HPC Sites**
    - **Between DoD HPC Sites**
  - **Frequency Of Changes Have Decreased**
  - **Remote Sites Are Often The Last To Be Told About Changes But The First To Be Affected By Them**
    - **IP Address Change At ERDC**
- **Firewalls**
  - **Impede File Transfer Capability**

Communications And Other Issues

- **File Transfers**
  - **HPC Allows Larger Calculations to Be Run**
  - **Data Files Grow With HPC**
  - **Bandwidth Does Not**
  - **Typical Data Files "Today" Are 4 Gbytes**
  - **File Transfer Time at 150 Kbytes/sec – 7.4 Hours**
  - **Greatly Inhibits 3D Visualization**
  - **Practically Prohibits Local Animation**
- **X-based Applications**
  - **Debuggers, Performance Analyzers, ...**
    - **Extremely Slow Updates**
- **Access To Training**
  - **Training Only Offered At Labs Or HPC Sites**

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Graphics Issues

- **Why 3D Graphics?**
  - **3D Visualization Of Static Images**
  - **More Natural Way To Look At Data**
  - **Humans Are Good At Pattern Recognition**
- **Why Animate?**
  - **Animations Provide Information About Data That Cannot Be Obtained From Static Images**
    - **Due To The Additional Time Dimension**
  - **Animation Types**
    - **Static Or Constant Time**
    - **Dynamic Or Time Varying**
  - **Animations Require A Considerable Amount Of Data**

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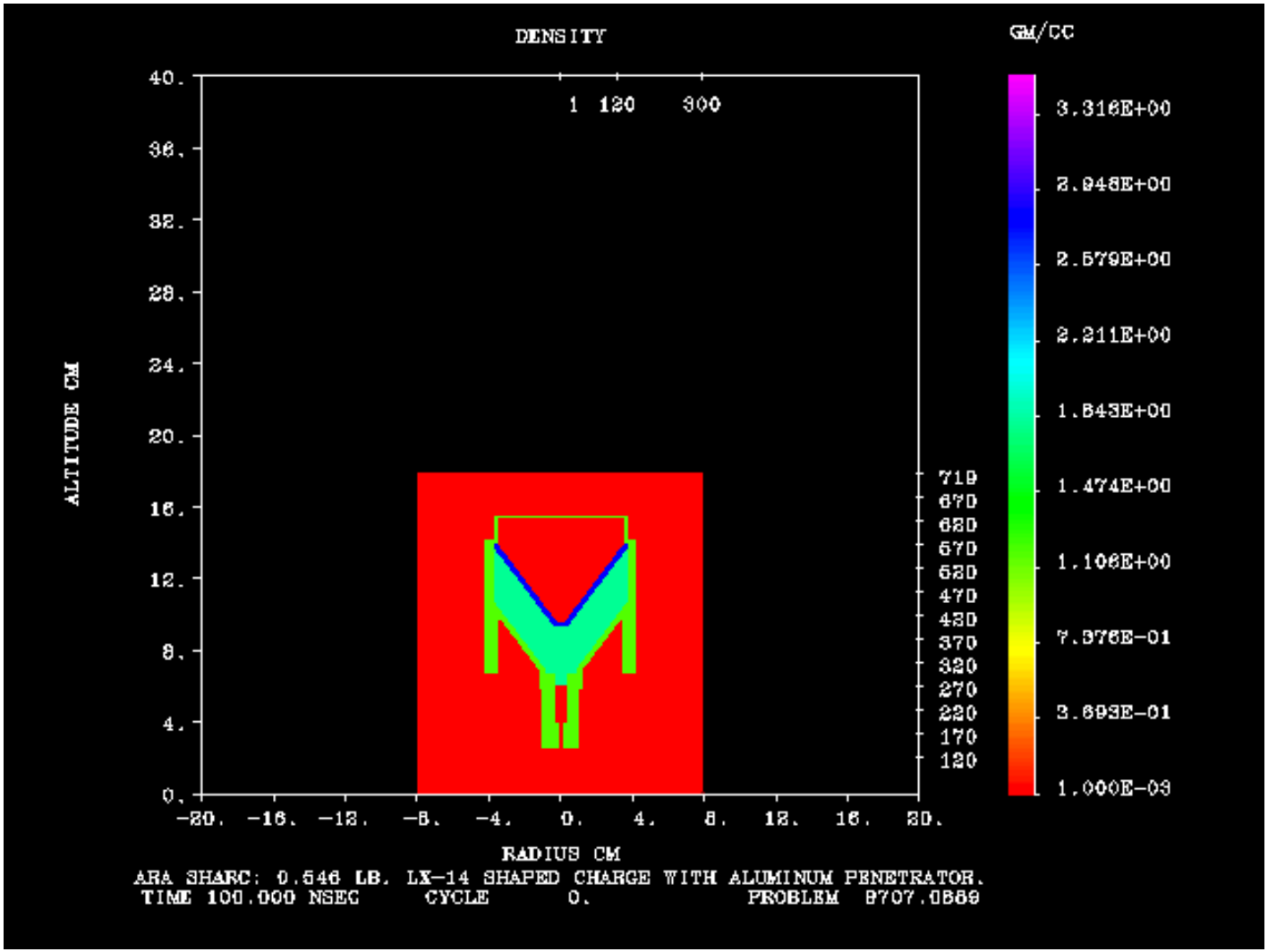
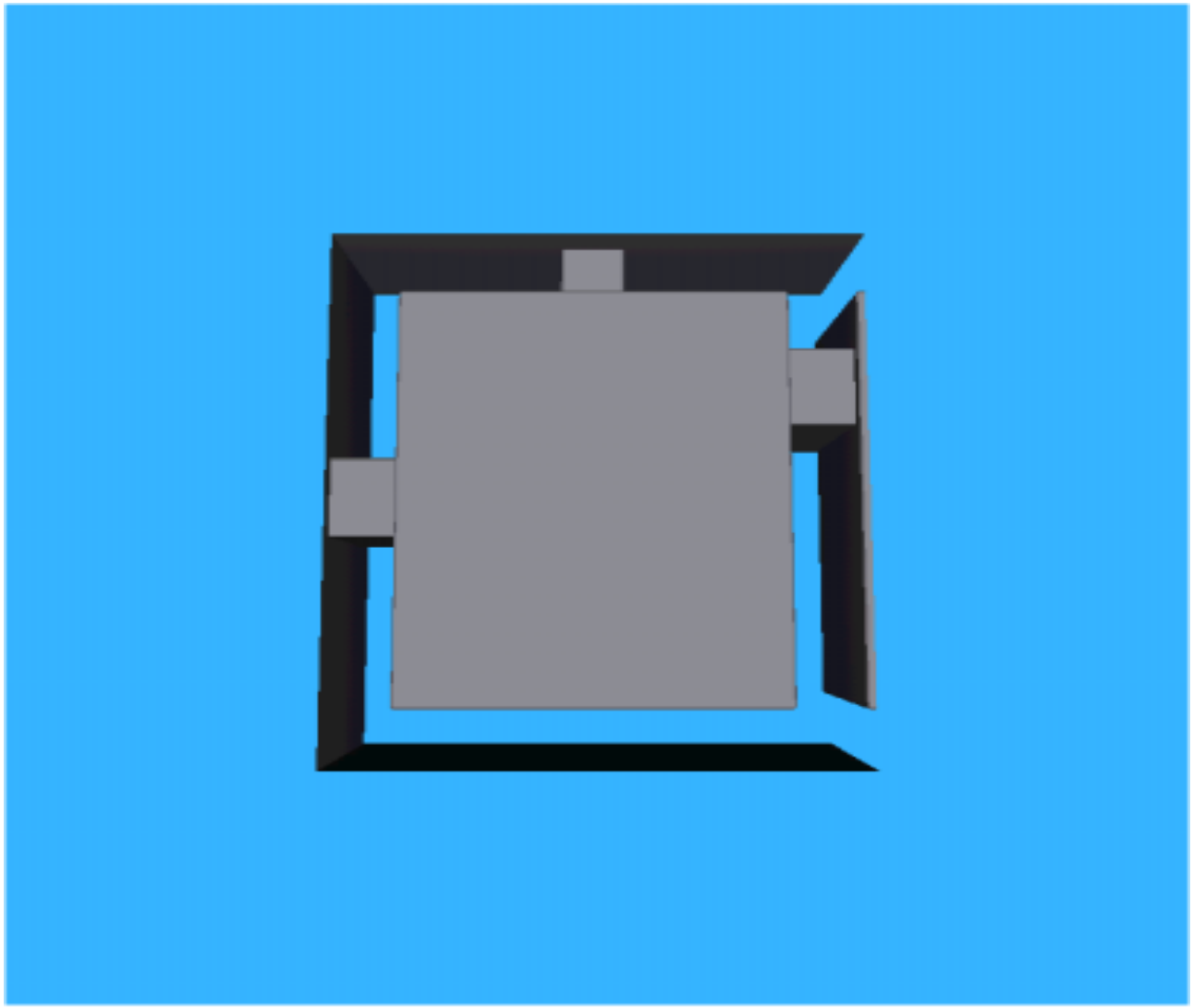
Graphics Issues

- **Making Animations With On-site Graphics Teams**
  - **ERDC Experience**
  - **Communications Difficulties**
  - **Delay Time Between Image Production And Viewing Results**
  - **Overall Results Have Been Good**

2D Animation Example



3D Constant Time Animation



Local Animation Process

- Reduce Data Set
- Compress Files
- Transfer Files
- Uncompress Files
- Make Animation
- Hope You Picked The Right Data

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Local Animation Example

SHAMRC Simulation of Non-Ideal Airblast Loading on T72 Tank

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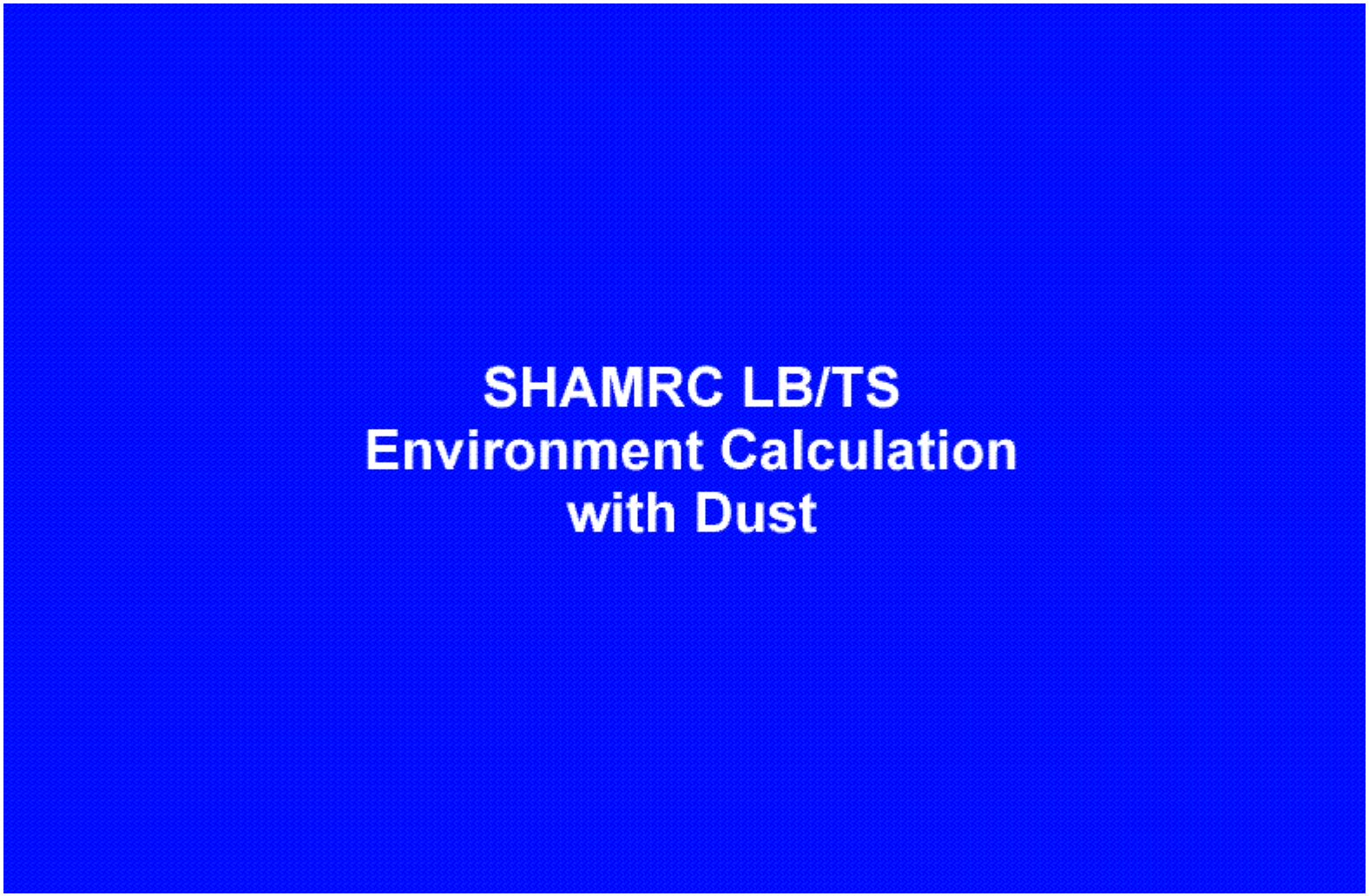
Local Animation Example



Remote Animation Process

+ **Make Data Files Available To Graphics Team**
+ **Discuss Your Vision Of What The Movie Should Look Like**
+ **Remote Graphics Team Produces Animation**
+ **Review The Animation**
+ **Iterate On Above 3 Steps (About 20 Times)**
+ **View The Final Product**

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Remote Animation Example

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Local Versus Remote Animation

- **Local Versus Remote Capabilities**
  - **Hardware**
  - **Software**
  - **Artistic**
- **Trade-off Between Time Spent Transferring Files and Animating Versus Time Spent Consulting Graphics Team**
- **Batch Processing Capability (and a Faster Connection) May Make A Combination Of Remote And Local Animation Feasible**

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Balancing Hardware and Software

- Hardware Advancing at a Faster Pace Than Software
- Requirements for the Latest, Fastest Platform Means Software Support Suffers
- Disconnect Between Same Vendor at Different Sites
  - LANL SGI O2K and ERDC SGI O3K
    - File System Problems
  - ERDC and ASC Compaq
    - LSF Problems

Summary

+ **NEED HIGH SPEED COMMUNICATIONS BETWEEN REMOTE AND HPC SITES**
  - **Keep Pace With Problem (File) Size Growth**

+ **New Systems Need to Be Thoroughly Checked Out Before Being Brought up in "Production" Mode**
  - **Longer Pioneer Access Periods**
  - **Better Response Time to Reported Problems**
  - **Direct Communication Between Users and System Administrators**

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